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END TO END SIMULATIONS OF ANTIPROTON TRANSPORT AND DEGRADATION

S. Padden† [1], E. Kukstas[1], P. Pusa, V. Rodin[1], C. P. Welsch[1]
University Of Liverpool, Liverpool, United Kingdom
K. Nordlund, University of Helsinki, Helsinki, Finland
[1]also at The Cockroft Institute, Daresbury, United Kingdom

Abstract

The ELENA ring decelerates anti-protons to 100 keV down from 5.3 MeV with transport to experiments handled by electrostatic transfer lines. Even at 100 keV antiprotons are still too high in energy for direct injection into an ion trap, and this is why degrader foils are used to further lower the energy. This paper presents full end-to-end simulations from the point of extraction until passing through the foil. This is achieved using realistic beam transport simulations coupled with accurate simulations of degrader foils via the use of density functional theory and molecular dynamics. Particles are tracked from the point of extraction until their injection into the trap with full physical modelling at all time steps. The results of this study provide a versatile platform for the optimization of low energy ion experiments towards specific targets.

INTRODUCTION

In light of recent advancements in the cooling of anti-hydrogen [1] it has become more important than ever to have a more complete understanding of the capture process of the anti-protons provided via the AD-ELENA (Antiproton Decelerator - Extra Low ENergy Antiproton) complex. Although ejected from the ELENA ring at 100 keV, this still remains too high for optimum trapping efficiency. Following deceleration in the ELENA ring antiprotons ($\bar{p}$) ejected from the ring travel through electrostatic beam lines towards various different experiments. At the point of exchange between the beam line and experiment a degrader foil is commonly used to bring the energy down even further in a manner destructive to the beam quality, but necessary for the trapping process. Throughout this study, specific focus is drawn onto the ALPHA (Antihydrogen Laser Physics Apparatus) catching trap, due to the presence of 5 kV end cap electrodes in the Penning-Malmberg trap, which gives a benchmark figure of 5 keV for optimum trapping [2]. Coupled with this requirement on energy is also a need for a better understanding of particle distribution upon leaving the foil, both in terms of spacial distributions and direction of travel.

Previous studies have focused on the usage of Monte Carlo simulations relying heavily on Binary Collision Approximation methods (BCA) [3, 4], which whilst successful do not account for the differences in stopping power seen between protons (p) and antiprotons ($\bar{p}$) of the same energy.

† Spadden@liverpool.ac.uk

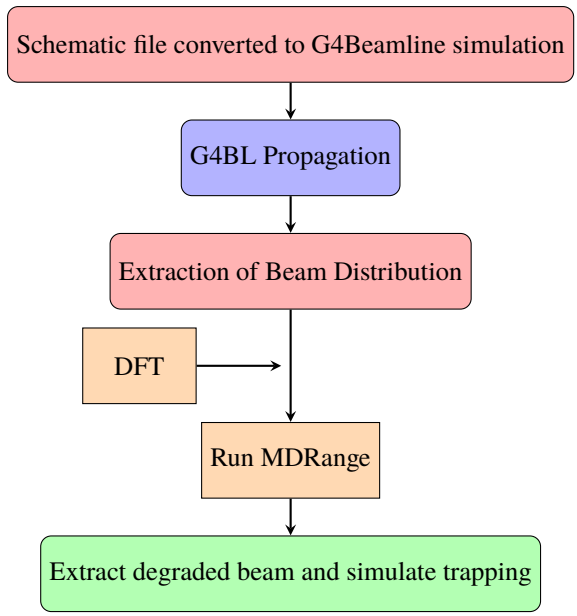

Figure 1: Flow chart describing the end to end simulation process, starting from initial schematic files through transport simulation, degradation and the early trapping process.

This paper outlines a more rigorous method of handling antiproton simulation allowing for deeper understanding of the destructiveness of degrader foils as a direct result of bunch parameters following transport. Complete end to end tracking is presented from the point of ejection from ELENA, until interaction with the degrader foils via transfer along electrostatic transfer lines implemented within G4Beamline [5]. Upon interaction with the foil, a quantum realistic simulation from density functional theory (DFT), using the simulation package ORCA [6], is implemented in the form of a screened coulomb potential into the molecular dynamics (MD) code MDRange [7]. This allows for the handling of complex trajectories and addresses some of the issues encountered by more traditional methods by accurately following $\bar{p}$ through its traversal of the foil bulk.

SIMULATION OVERVIEW

Figure 1 shows the complete simulation procedure. By following the above method a particle can be considered to be fully tracked and modeled from the moment of injection until capture by the trap. DFT calculations must be done outside of the simulation path as they require manual adjustment for each specific case. The schematic file in discussion is

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in the .SVG format, a widely used vector graphic image style allowing for an accurate schematic model. A code has been developed and will be made widely available[1] upon completion to take .SVG file schematics and convert directly into a G4Beamline simulation. Following conversion, the simulation is run for published ELENA parameters [8] and processed until the point of interaction with the ALPHA degrader foil. Upon reaching the foil, bunch parameters are extracted and subsequently modify the MDRange input files accordingly. With bunch parameters and force fields from DFT simulations MDRange can accurately simulate $\bar{p}$ movement in the foil. The MDRange output is extracted and reinserted into a further G4Beamline simulation of the ALPHA catching trap.

Anti-Proton Transport

To simulate the dynamics of $\bar{p}$ travelling from ELENA up to the foil, G4Beamline is implemented into the simulation. G4Beamline is an outer wrapper of Geant4 and as such contains accurate electromagnetic modelling of commonly used accelerator components with accurate physical processes. To simulate the transfer through electrostatic beam lines used within the AD-ELENA complex, adjustments had to be made to the source code of G4Beamline, a more detailed breakdown of this method is found in [9]. These include implementation of electrostatic quadrupoles with field definition based on the experimental measurements [10], new tracking methods and realistic description of bending elements.

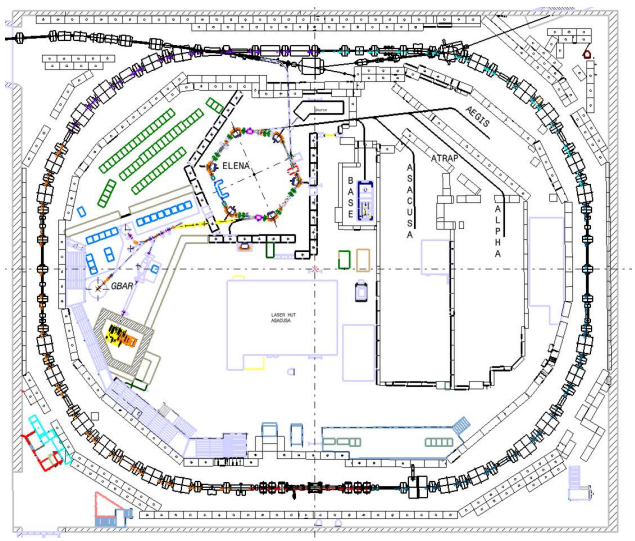

Figure 2: Schematic Layout of the AD-ELENA complex located within CERN. Reproduced from [11].

Figure 2 is a schematic layout of the AD-ELENA complex. The current simulation path is from ELENA along the transfer lines to the ALPHA trap. Upon reaching the foil the simulation terminates and returns the beam distribution at point the of contact as shown at Fig. 3. Future studies will accurately link the spacial beam distribution, spread and energy directly into MD simulations of the foil. As G4Beamline handles beams in 6D space, extraction of the required parameters for MD simulations is handled in a simple manner: a singular code handles the complete schematic to the MD simulation, limiting the need for user interaction.

Degrader Foil Simulations

An accurate simulation of $\bar{p}$'s passing through matter requires handling of complex trajectories about nuclei and subsequent interactions within the foil. Previous BCA simulation methods do not differentiate between matter and antimatter. Of particular note is the way in which electrons differ in their interaction between protons and antiprotons.

To account for this it is first necessary to implement DFT simulations to gather detailed force fields for the interactions between $\bar{p}$ and an atomic material of choice, both protons and antiprotons have been simulated in this way. By iteration across multiple inter particle distances a discrete distribution can be built showing the differences between matter and antimatter. For protons the expected Lennard-Jones potential is observed whilst for antiprotons a purely attractive potential is calculated, immediately outlining the need for a more detailed handling than previous BCA codes as trajectories now can be more complex than in previously used elastic collision methods.

DFT simulations are undertaken using second order Møller–Plesset perturbation theory [12] on triple polarized def2-TZVP basis sets [6] to model the Hartree-Fock electron wave function of the foil material in question, this ensures good convergence. It is expected that closed shell atomic systems will exhibit less screening than those with "free" outer electrons due to reduced quadrupole coupling. Figure 4 shows inter-particle potential energies as a function of distance and is produced by iteration from ORCA. As expected the filled outer electron orbital in Neon exhibits significantly lower interaction than Silicon.

By fitting and normalising the distribution in Fig. 4 a screening function, $\Phi(r)$, can be produced which modifies the pure Coulomb potential to give a more accurate reflection of the force field between the $\bar{p}$ and atom pair:

$$V(r) = \frac{\Phi(r)}{4\pi\epsilon_0}\frac{Z_1 Z_2 e^2}{r}, \tag{1}$$

whereby $V(r)$ is the potential energy as a function of distance, $Z_1, 2$ are the respective atomic charges, e is the electron charge, ϵ_0 retains its usual meaning as the permittivity of free space

Through subsequent fitting algorithms this can be built into a continuous distribution, allowing for usage within molecular dynamics simulations. Although multiple molecular dynamics simulation programs exist, few are capable of handling particles with appreciable momentum and complex orbit trajectories. For this reason MDRange was selected as it has been proven in the past to work successfully for

[1] Please contact author to request code before release

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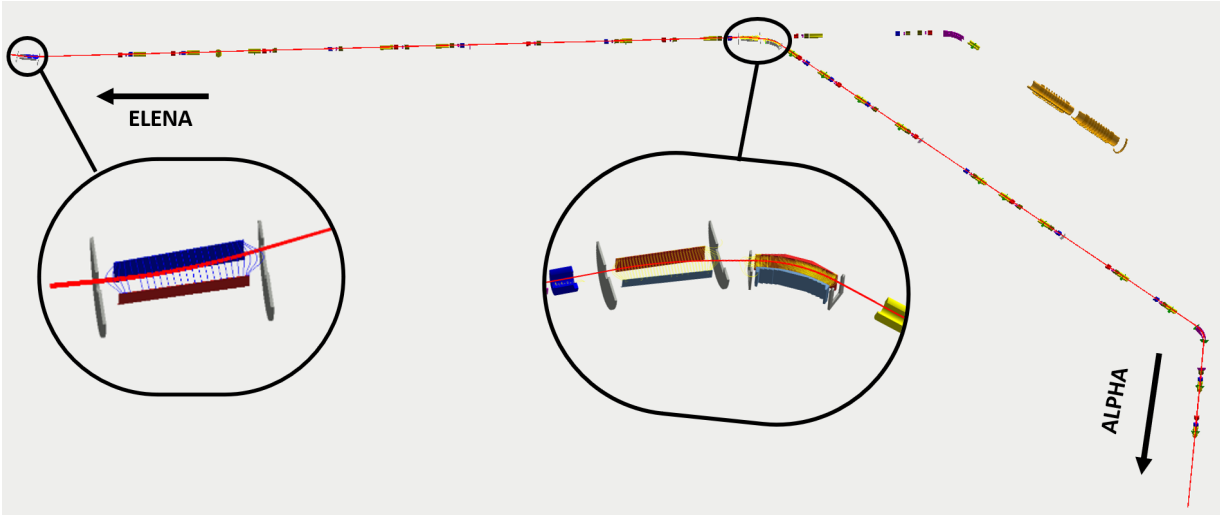

Figure 3: Beam transport to the ALPHA experiment simulated in G4Beamline (cut in half). Fast deflector from ELENA ring and two deflectors to ALPHA branch are highlighted. Field lines are partially visualized. Electrode color corresponds voltage polarity with respect to charge of the beam as negative (red).

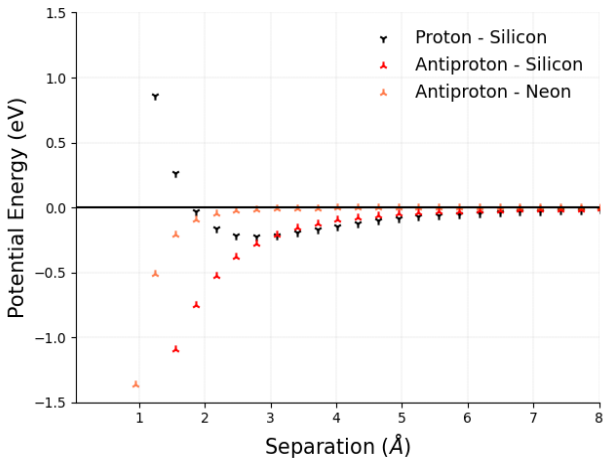

Figure 4: DFT Calculations of proton and antiproton interaction energy with Silicon, and antiproton with Neon, as a function of separation distance.

the simulation of matter-antimatter interactions [13]. By using DFT-created force fields as screening functions with MDRange, Eq. (1) can be accurately modelled for various different foil materials. These materials are presented as a crystalline material with a repeating lattice structure for a desired Z depth (direction of beam travel) and assumed infinite X-Y plane (perpendicular to beam travel). Given the parameters of ELENA are well simulated, this can be considered a reasonable assumption providing the foil has been accurately mounted.

SUMMARY AND OUTLOOK

A simulation outline has been presented which will calculate accurate forces experienced between antiprotons and nuclei in a degrader foil. By simulating antiproton transport along the beam lines, the beam parameters at the point of contact are coupled with antimatter-matter force fields to produce a realistic molecular dynamics simulation which allows for complicated traversal paths through the foil.

Future plans involve the extraction of data from MDRange simulations at the back of the foil and reintegration into a G4Beamline simulation of the trap capture process to measure the trapping efficiencies of multiple foils. By using multiple DFT and MD simulations for an assortment of foil and compound foils, accurate input beam distributions and realistic early trapping simulations, future work will demonstrate the efficiency changes as a direct result of degrader foil selection.

The program currently in development to allow rapid conversion of schematic style images directly into accurate accelerator models built within G4Beamline will allow experimental users to quickly gain beam information without the need for custom-written simulation codes.

This work however is not limited to degrader foils and beam line simulations, a deeper understanding of the transport of $\bar{p}$ in bulk material is necessary for future medical treatments. Should the straggling prove to significantly differ from protons, then aiming $\bar{p}$ at targets within the human body will require deeper analysis.

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